

(3,3,3-²H₃)Propan-1-ol
61844-01-7 | DTXSID50480196

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.89	0.25	0.88	0.26	0.75	0.38

Model Results

Predicted value: 4.43 days

Global applicability domain: Outside

Local applicability domain index: 3.44e-01

Confidence level: 7.64e-01

Nearest Neighbors from the Training Set

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2-Methylhexane

Measured: 12.5

Predicted: 5.54

Image not found

2-Methylheptane

Measured: 12.5

Predicted: 3.99

Image not found

2-Methyloctane

Measured: 40.7

Predicted: 4.23

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Tetradeca-1,13-diene

Measured: 367

Predicted: 8.69